

Controlled hole doping of a Mott insulator of ultracold fermionic atoms

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Considering a system of ultracold atoms in an optical lattice, we propose a simple and robust implementation of a quantum simulator for the *homogeneous* t - J model with a well-controlled fraction of holes x . The proposed experiment can provide valuable insight into the physics of cuprate superconductors. A similar scheme applied to bosons, moreover, allows one to investigate experimentally the subtle role of inhomogeneity when a system passes from one quantum phase to another.

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Gases of ultracold atoms in optical lattice potentials provide extremely clean and controllable conditions for studying strongly correlated many-body physics [1]. Since for deep lattices these systems are described quantitatively by Hubbard-type Hamiltonians [2], they have great potential to serve as quantum simulators [3] for paradigmatic models of condensed matter physics. This prospect is fed by results for bosonic systems. In a seminal experiment, the quantum phase transition from a superfluid of bosons to a strongly correlated Mott insulator—predicted for the bosonic Hubbard model [4]—has been observed [5]. Moreover, quantitative agreement between experiment and *ab initio* quantum Monte Carlo simulations clearly confirm the validity of the Bose-Hubbard description [6].

While the elementary Hubbard model for bosons is rather well understood, this is not the case for repulsively interacting fermions: In a Mott insulator, with interaction localizing one particle of “spin” $s = \uparrow$ or \downarrow at each site, Fermi statistics gives rise to an *antiferromagnetic* superexchange coupling J between neighboring spins. Intriguing physics is expected when such a quantum antiferromagnet is frustrated, either by a non-bipartite lattice geometry [7] or by doping it with holes (or fermions) displacing spins when moving around [10]. The latter scenario for a square lattice is conjectured to give rise to $d_{x^2-y^2}$ -wave pair superfluidity and to explain basic properties of high-temperature cuprate superconductors [8–10]. However, conclusive theoretical evidence of whether the plain Hubbard physics supports a superconducting state is still lacking. As pointed out already in Ref. [11], here a cold atom realization of the fermionic Hubbard model (or its descendant, the t - J model) could provide critical insight.

The recent observation of a Mott insulator of repulsively interacting fermionic atoms in a deep optical lattice [12] is an important first step toward a clean cold atom realization of strongly correlated fermionic Hubbard physics. However, further steps in that direction require solutions to two problems: (i) The temperatures

that can be achieved presently are still larger than (or at most comparable to) the energy scale of the superexchange spin-spin coupling [13]. Promising novel cooling procedures have been proposed to tackle this problem [14] (cf. also [15]). (ii) While it is relatively easy to create an incompressible Mott region with one atom per site in the center of a parabolic trap, it is very hard to dope such a trapped Mott insulator in a controlled way. When the particle number in the center of the trap is lowered, e.g. by slowly widening the trap, the central Mott-insulator phase will not be doped with holes homogeneously. Rather, it will melt from the edge. Also simply switching off the trapping potential (i.e. compensating it with a blue-detuned laser) is difficult, since then particles may leak out and it will be hard to control the lattice filling. In this Rapid Communication we propose a robust solution to problem (ii). Our method allows one to both accurately control the fraction x of hole doping and effectively compensate the trapping potential. Both are crucial in order to learn about high-temperature superconductivity with ultracold atoms. Applied to bosons, our scheme, moreover, allows one to experimentally investigate the non-trivial influence of spatial inhomogeneity when a system passes from one quantum phase to another [16].

Our basic idea is to create holes in a fermionic Mott insulator by adding auxiliary bosonic particles to the system that interact repulsively both with the fermions and with each other. Each boson repels a fermion from one site. Experimentally, one has to create a mixed Mott phase with one particle, either fermion or boson, per site. This spatially rather well-defined “simulator region” resembles the system to be simulated. The degree of hole doping is well controlled by the number ratio between bosons and fermions. The price to be payed is that, unlike the tunneling of a real hole, the motion of the bosons happens via boson-fermion swaps, being slow second-order superexchange processes (cf. [17, 18] for the case of “spinless” Bose-Fermi mixtures). But this type of hole kinetics brings also a great advantage: Consider the trap being very similar for fermions and bosons (think of two Ytterbium isotopes in a far off-resonant dipole potential). Then such a boson-fermion swap on two neighboring sites will change the potential energy only marginally, even if

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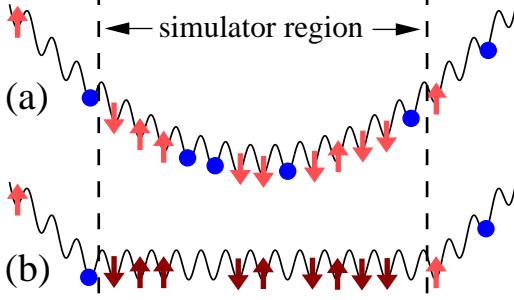


FIG. 1: (color online) (a) Sketch of the lattice and trapping potential felt by both fermions and bosons. Assuming strong on-site repulsion and symbolizing fermions by light red arrows and bosons by blue bullets, an occupation snap shot is sketched. There is a central mixed Mott region, the simulator region, with one boson or fermion per site. (b) In the simulator region, fermions move by fermion-boson swaps not changing potential energy. Here a description solely in terms of a new type of fermions (dark red arrows) is possible, with bosons implicitly taken care of as holes. These fermions move with an effective tunneling amplitude and do not feel the trap; the fraction x of holes equals that of bosons.

the trapping potential does change between both sites. Hence, within the simulator region the physics is hardly influenced by the trap, cf. Fig. 1. Below we will show that this region is accurately described by the *homogeneous t-J* model with *controlled hole fraction* x . The *t-J* model [19] (cf. [20] for other cold atom applications) describes the doped fermionic Mott-insulator, with fermion hopping t and superexchange spin coupling J ($\approx t/3$ in cuprates [21]). Second-order superexchange is crucial for the physics of the doped fermionic Mott-insulator. We want to emphasize that our proposal, in which both spin coupling and hopping originate from superexchange, does not involve any process above second order. Our scheme is, in a sense, contrary to the slave-boson approach to the *t-J* model (where auxiliary bosons describing holes are introduced as a purely theoretical concept): We propose a physical system of real bosons and spin 1/2 fermions that behaves as a system of fermions alone.

Before presenting the details of our proposal, we want to mention that recently another, interesting solution to problem (ii) of controlled hole doping [not to the issue of temperature, problem (i)] has been proposed [22]: The authors suggest realizing an attractive Hubbard model, which for a bipartite lattice can be mapped to a repulsive one (see, e.g., [23]). In particular, an imbalance of \uparrow and \downarrow fermions for attractive interaction, being relatively easy to control experimentally, corresponds to hole or particle doping in the repulsive model. Unfortunately, at the same time, the trap felt by the attractive fermions transforms to an inhomogeneous magnetic field, favoring a spatial separation of repulsive \uparrow and \downarrow fermions.

Let us now describe in detail our approach to controlled hole doping. We consider a mixture of $N_f \equiv N_\uparrow + N_\downarrow$ fermionic and N_b bosonic atoms ($N \equiv N_f + N_b$) in an op-

tical lattice, with the fermions having equally populated “spin” states $s = \uparrow, \downarrow$. The system is described quantitatively by the Hubbard model [2]

$$\begin{aligned} \hat{H}_{ffb} = & - \sum_{\langle i,j \rangle} \left[\sum_{s=\uparrow,\downarrow} t_{ij}^f (\hat{f}_{is}^\dagger \hat{f}_{js} + \text{h.c.}) + t_{ij}^b (\hat{b}_i^\dagger \hat{b}_j + \text{h.c.}) \right] \\ & + \sum_i [U^{ff} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + U^{fb} \hat{n}_{if} \hat{n}_{ib} + \frac{U^{bb}}{2} \hat{n}_{ib} (\hat{n}_{ib} - 1)] \\ & + \sum_i [V_i \hat{n}_i + \delta V_i \hat{n}_{if}]. \end{aligned} \quad (1)$$

Here \hat{f}_{is}^\dagger and \hat{b}_i^\dagger denote creation operators for fermions and bosons at site i . We also define number operators $\hat{n}_{is} \equiv \hat{f}_{is}^\dagger \hat{f}_{is}$, $\hat{n}_{ib} \equiv \hat{b}_i^\dagger \hat{b}_i$, $\hat{n}_{if} \equiv \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, and $\hat{n}_i \equiv \hat{n}_{if} + \hat{n}_{ib}$. The first line of Eq. (1) comprises fermion and boson tunneling between neighboring sites, with positive matrix elements t_{ij}^f and t_{ij}^b (depending exponentially on lattice depth [2]). The second line takes care of the repulsive on-site interaction between the different types of particles, with Hubbard energies U^{ff} , U^{fb} , and U^{bb} (weakly depending on lattice depth and being proportional to the corresponding s -wave scattering lengths [2]). Finally, the third line includes co-centric trapping potentials $V_i^f \equiv V_i + \delta V_i$ and $V_i^b \equiv V_i$ for fermions and bosons [$V_i^f \equiv V_i^b \equiv 0$ in the center], with δV_i to be tuned small.

We are interested in the parameter regime giving rise to an extended mixed Mott region, with one particle (boson or fermion) per site, in the center of the trap. We assume a cubic lattice of spacing d with site locations $d\mathbf{r}_i$, as well as a parabolic confinement $V_i = \frac{1}{2}\alpha r_i^2$. We also define both $U_{\min} \equiv \min(U^{ff}, U^{fb}, U^{bb})$ and $t_{\max} = \max(\{t_{ij}^f\}, \{t_{ij}^b\})$. Temperatures are well lower than t_{\max} . Now, $t_{\max} \ll U_{\min}$ and $\mu < U_{\min}$ (while $t_{\max} \ll U_{\min} - \mu$), with chemical potential μ , guarantees strong suppression of double occupancy. On the other hand, the trap V_i prevents vacancies from entering the central region: the occupied region of radius $\rho \approx (3N/4\pi)^{1/3}$ features only a thin shell (a few d wide) of reduced particle number, provided $t_{\max} \lesssim \alpha\rho \equiv \Delta V_{\text{edge}}$, where ΔV_{edge} is the energy difference between sites at radius ρ and $\rho + 1$. With the above requirements fulfilled, the chemical potential for bosons and fermions is basically given by the potential energy needed to place a particle at the edge of the occupied region, $\mu \approx \frac{1}{2}\alpha\rho^2$. One has $\Delta V_{\text{edge}}/\mu = 2\rho$. The radii ρ might range from 10 to 30. All in all, $t_{\max} \lesssim \Delta V_{\text{edge}} \ll \mu < U_{\min}$ summarizes the parameter regime assumed here. In practice, t_{\max}/U_{\min} can be adjusted via the lattice depths, while μ/U_{\min} can be tuned to a value of 1/2, say, by varying the trap depth α .

In the bulk of the mixed Mott region, at each site i , strong repulsion in combination with the trapping confinement V_i gives rise to the constraint

$$\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} + \hat{n}_{ib} = 1, \quad (2)$$

with the overall boson fraction $x \approx N_b/N$. The system

can be described by an effective Hamiltonian \hat{H}_{eff} acting in the subspace \mathcal{S}_1 defined by Eq. (2). Treating the first line of \hat{H}_{ffb} as perturbation \hat{H}_1 , we can expand \hat{H}_{eff} according to degenerate perturbation theory.¹ Up to second order, using $\hat{n}_{ib} = 1 - \hat{n}_{if}$ in \mathcal{S}_1 , one finds

$$\begin{aligned} \hat{H}_{\text{eff}} = & \hat{P} \left\{ - \sum_{\langle ij \rangle} \sum_s t_{ij} (\hat{f}_{is}^\dagger \hat{b}_i \hat{b}_j^\dagger \hat{f}_{js} + \text{h.c.}) + \sum_i W_i \hat{n}_{if} \right. \\ & \left. + \sum_{\langle ij \rangle} \left[J_{ij} \left(\hat{S}_i \hat{S}_j - \frac{\hat{n}_{if} \hat{n}_{jf}}{4} \right) + U_{ij}^{nn} \hat{n}_{if} \hat{n}_{jf} \right] \right\} \hat{P}, \end{aligned} \quad (3)$$

where \hat{P} projects on \mathcal{S}_1 and where we have introduced the usual spin operators $\hat{S}_i \equiv \frac{1}{2} \sum_{s's} \hat{f}_{is'}^\dagger \boldsymbol{\sigma}_{s's} \hat{f}_{is}$ with Pauli matrices $\boldsymbol{\sigma}_{s's}$. Moreover,

$$t_{ij} \equiv 2 \frac{t_{ij}^f t_{ij}^b}{U^{fb}} [1 + \delta_{ij}^{fb}], \quad (4)$$

$$J_{ij} \equiv 4 \frac{(t_{ij}^f)^2}{U^{ff}} [1 + \delta_{ij}^{ff}], \quad (5)$$

$$U_{ij}^{nn} \equiv (I_{ij}^{fb} - I_{ij}^{bb}), \quad (6)$$

$$W_i \equiv \delta V_i + \sum_{j \in \text{adj}(i)} [I_{ij}^{bb} - I_{ij}^{fb}/2 - \delta I_{ij}^{fb}]. \quad (7)$$

with $\delta_{ij}^\nu \equiv [(\frac{U^\nu}{V_i - V_j})^2 - 1]^{-1}$, $I_{ij}^{bb} \equiv 4 \frac{(t_{ij}^b)^2}{U^{bb}} [1 + \delta_{ij}^{bb}]$, $I_{ij}^{fb} \equiv 2 \frac{(t_{ij}^f)^2 + (t_{ij}^b)^2}{U^{fb}} [1 + \delta_{ij}^{fb}]$, $\delta I_{ij}^{fb} \equiv \frac{(t_{ij}^f)^2 - (t_{ij}^b)^2}{U^{fb}} \delta_{ij}^{fb} \frac{U^{fb}}{V_i - V_j}$, and $\text{adj}(i)$ containing all sites adjacent to i . In Hamiltonian (3), t_{ij} describes boson-fermion swaps, i.e. effective fermion tunneling, W_i is the effective potential felt by fermions, J_{ij} stands for the usual fermionic antiferromagnetic superexchange coupling, and U_{ij}^{nn} captures boson-mediated nearest-neighbor interaction between fermions that can be attractive, repulsive or zero.

Hamiltonian (3) is equivalent to a t - J -type model, describing a purely fermionic system when strong repulsion suppresses double occupancy. This can be seen by introducing composite-fermion creation operators

$$\hat{c}_{is}^\dagger \equiv \hat{f}_{is}^\dagger \hat{b}_i. \quad (8)$$

We define $\tilde{n}_{is} \equiv \hat{c}_{is}^\dagger \hat{c}_{is}$ and $\tilde{S}_i \equiv \frac{1}{2} \sum_{s's} \hat{c}_{is'}^\dagger \boldsymbol{\sigma}_{s's} \hat{c}_{is}$. Using $\hat{P} \hat{f}_{is}^\dagger \hat{f}_{is} \hat{P} = \hat{P} \hat{f}_{is'}^\dagger (1 + \hat{b}_i^\dagger \hat{b}_i) \hat{f}_{is} \hat{P} = \hat{P} \hat{c}_{is'}^\dagger \hat{c}_{is} \hat{P}$, yields both $\tilde{n}_{is} = \hat{n}_{is}$ and $\tilde{S}_i = \hat{S}_i$ in \mathcal{S}_1 . Bosons transform to empty sites (holes) and \mathcal{S}_1 to the subspace defined by $\tilde{n}_i \leq 1$ with $\tilde{n}_i \equiv \tilde{n}_{i\uparrow} + \tilde{n}_{i\downarrow}$. Thus, we can rewrite \hat{H}_{eff} as t - J

Hamiltonian in terms of \hat{c}_{is}^\dagger -fermions alone:

$$\begin{aligned} \hat{H}_{\text{eff}} = & \hat{P} \left\{ - \sum_{\langle ij \rangle} \sum_s t_{ij} (\hat{c}_{is}^\dagger \hat{c}_{js} + \text{h.c.}) + \sum_i W_i \tilde{n}_i \right. \\ & \left. + \sum_{\langle ij \rangle} J_{ij} \left[(\tilde{S}_i \tilde{S}_j - \frac{\tilde{n}_i \tilde{n}_j}{4}) + U_{ij}^{nn} \tilde{n}_i \tilde{n}_j \right] \right\} \hat{P}. \end{aligned} \quad (9)$$

Transformation (8) (being inverse to a the slave-boson transformation) is illustrated in Fig. 1.

The t - J model (9) with $W_i = \text{const.}$, $U_{ij}^{nn} = 0$, $t_{ij} = t$, $J_{ij} = J \approx t/3$, and boson fraction x , is the most simple candidate to explain high-temperature cuprate superconductivity [8–10, 21]. The fermion-boson mixture considered here, allows one to realize these parameters quite accurately: Starting from a cubic lattice, the tunneling amplitudes t_{ij}^f and t_{ij}^b can be suppressed in one direction by ramping up the lattice in that direction, leading to a stack of uncoupled square lattices layers. From now on, we will only consider the intra-layer physics. Creating the optical lattice by using a rather broad laser beam, within the occupied region of the trap (created by further beams) the lattice will be practically homogeneous. Thus, $t_{ij}^f \simeq t^f$ and $t_{ij}^b \simeq t^b$. Furthermore, potential differences $|V_i - V_j|$ between neighboring sites are much smaller than U^{ff} , U^{fb} and U^{bb} , giving $\delta_{ij}^\nu \lesssim 10^{-3}$ ($\nu = ff, fb, bb$) for the parameters estimated in a previous paragraph. With that the model parameters (4)–(6) are to good approximation homogeneous within the simulator region, $t_{ij} \simeq t$, $J_{ij} \simeq J$, and $U_{ij}^{nn} \simeq U^{nn}$. By the very same arguments, also the last three terms contributing to W_i [Eq. (7)] have a negligible spatial dependence compared to the effective hopping parameter t , being the relevant energy scale here. Thus, if also the difference between boson and fermion potential δV_i is smaller than t , one achieves a practically flat effective potential $W_i \simeq W$, without fermions leaking out of the system, cf. Fig. 1(b).

In an experimental realization, the hole fraction x is controlled by the boson fraction (also amenable to postselection). Moreover, $t/J \simeq \tau u_f/2$ and $U^{nn}/J \simeq [2u_b^{-1} - \tau^{-2} - 1]u_f/2$, with $\tau \equiv t^b/t^f$ and $u_\nu \equiv U^{\nu\nu}/U^{fb}$ ($\nu = f, b$), can be tuned by using Feshbach resonances and by modifying the lattices for bosons and fermions, either in depth or relative position. A candidate system is a mixture of Ytterbium isotopes [25–27]: The total angular momentum of Yb is just given by the nuclear spin I , not influencing the interparticle interaction. A mixture of two spin states of fermionic ^{173}Yb ($I = 5/2$) with bosonic ^{168}Yb or ^{174}Yb (both $I = 0$) is described by three positive s -wave scattering lengths, with $a_{ff}/a_{fb} = 5.2$ (1.4), $a_{bb}/a_{fb} = 6.5$ (0.8) and $a_{fb} = 2.0\text{nm}$ (7.3nm) for ^{168}Yb (^{174}Yb) [26]. Also optical Feshbach resonances are available [27]. Using a far off-resonant optical potential allows one to create practically equal traps for bosonic and fermionic isotopes without fine-tuning. Considering the Mott regime, according to band structure calculations, typical Hubbard interaction parameters for Yb will roughly be on the order of 10 kHz. The effective tunneling matrix element t will be about 200 times

¹ With unperturbed states $a, a' \in \mathcal{S}_1$, $b \notin \mathcal{S}_1$ and energies $E_a, E_{a'}, E_b$, the leading orders of \hat{H}_{eff} read [24]: $\langle a' | \hat{H}_{\text{eff}}^{(0)} | a \rangle = \langle a' | \hat{H}_0 | a \rangle$, $\langle a' | \hat{H}_{\text{eff}}^{(1)} | a \rangle = \langle a' | \hat{H}_1 | a \rangle$, and $\langle a' | \hat{H}_{\text{eff}}^{(2)} | a \rangle = \sum_b \langle a' | \hat{H}_1 | b \rangle \langle b | \hat{H}_1 | a \rangle \frac{1}{2} [(E_a - E_b)^{-1} + (E_{a'} - E_b)^{-1}]$.

smaller. Such low energy scales are challenging experimentally. However, they are not very specific to our proposal, but rather are a generic consequence of the fact that the t - J physics is inevitably the physics of superexchange processes. Therefore, the temperatures needed here are only moderately lower than those that would be needed in an experimental setup where—somehow—a Mott insulator of fermionic atoms can be doped with real holes in a controlled fashion. While in the latter case $U^{ff}/t^f \gg 1$ would be required, in our proposal one has $U^{ff}/t^f \gg 2(t/J) \approx 6$ (combine $\tau_{uf} \simeq 2t/J$ and $U^{fb} \gg t^b$), reducing J by a factor of 6 only.

At hole doping $x \lesssim \mathcal{O}(0.01)$ and temperatures $k_B T \lesssim J$, the homogeneous t - J model (9) is known to give rise to (quasi-)long-range antiferromagnetic Néel order. At larger doping $x \sim \mathcal{O}(0.1)$ and even lower temperatures, the model is conjectured to possess yet another ordered phase, namely the $d_{x^2-y^2}$ -wave superconducting one observed also in the cuprates [9, 10]. Superfluidity of \hat{c} -fermions (that is in the t - J model) is connected to superfluidity of *both* \hat{f} -fermions and \hat{b} -bosons [28]; both have to be probed. The bosonic superfluidity is related to a (quasi)condensate at quasimomentum $\mathbf{k} = 0$, visible in time-of-flight absorption images.² In order to verify d -wave superfluidity of the fermions one can resort to different schemes for measuring quasiparticle excitations (as well as their interference) that have been proposed for cold atom systems for this purpose [11, 29].

In the cuprates, at optimal doping, superconducting behavior appears at temperatures that are at least one order of magnitude smaller than J [10, 21]. It is challenging to achieve these temperatures with cold atoms, and novel cooling techniques, as those proposed in Refs. [14], have to be implemented. The system has to be divided into a low-entropy part (lacking low-lying excitations) and a part carrying most of the entropy (a metallic shell or a boson-gas reservoir). The latter is removed before the system is adiabatically transferred into the desired state. In our fermion-boson system, a suitable gapped low-entropy phase would be an insulator of two fermions and an integer number of bosons at each site, to be created by making the trap steep and the lattice deep.

Finally, we would like to mention that neutralizing the trapping potential the way described here is also possible and interesting for bosons. In Refs. [16] it has been shown

² Bosons and \uparrow and \downarrow fermions can be imaged separately by selective absorption or Stern-Gerlach separation.

that the presence of a trap can fundamentally change the nature of the transition between an insulating and a superfluid quantum phase. The reason is not that the trapped system is too small to sharply distinguish between the two phases. It is more subtle: Because of the inhomogeneity, the transition occurs locally by displacing the interface separating spatial regions of different bulk phases. However, this spatial interface might be a smooth crossover rather than a sharp transition. A direct consequence can be that the adiabatic passage between two quantum phases is greatly facilitated by the trap. A simple lattice model that would allow to study such phenomena is given by spinless hard-core bosons on a square lattice with nearest-neighbor repulsion U_{nn} and hopping t . It features a transition from a checkerboard insulator at half filling and small t/U_{nn} to a superfluid phase [30]. The model (being equivalent to an XXZ spin 1/2 model) can be realized experimentally by creating a mixed Mott insulator having one boson of either species $s = 1$ or 2 on each site [17]. Mapping $\hat{b}_i^\dagger \equiv \hat{b}_{i1}^\dagger \hat{b}_{i2}^\dagger$, the system is described by a single type of hard-core boson only, with $U_{nn} = (t_1^2 + t_2^2)/U_{12} - 4t_2^2/U_{22}$, $t = 2t_1 t_2 / U_{12}$ and residual trapping potential $W_i = V_{i1} - V_{i2}$. Here $U_{ss'}$, t_s , and V_{is} denote on-site interaction, tunneling, and traps for the species $s = 1$ and 2. Now W_i can be tuned constant without making particles leak out. Thus, a ramp of t/U_{nn} at different rates can now be performed both with and without parabolic potential, and the degree of adiabaticity in passing the transition can be compared.

We have proposed a robust implementation of a quantum simulator for the homogeneous t - J model with well controlled hole doping, using a sample of ultracold bosonic and fermionic atoms in an optical lattice. We believe that—once the necessary temperatures are realized—our scheme can serve to gain crucial insight into the physics of strongly correlated quantum matter. Moreover, realizing a *homogeneous* bosonic system allows one to investigate experimentally the role of inhomogeneity when passing from one quantum phase to another.

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